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Abderrafi M. Ougouag
Joshua M. Cogliati
Jan-Leen Kloosterman

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METHODS FOR MODELING THE PACKING OF FUEL ELEMENTS IN PEBBLE BED REACTORS

Abderrafi M. Ougouag, Joshua J. Cogliati
Idaho National Laboratory
PO Box 1625, Idaho Falls, ID 83415-3885
Abderrafi.Ougouag@inl.gov Joshua.Cogliati@inl.gov

Jan-Leen Kloosterman
Delft University of Technology
Mekelweg 15, NL 2629 JB Delft, The Netherlands
kloosterman@iri.tudelft.nl

ABSTRACT

Two methods for the modeling of the packing of pebbles in the pebble bed reactors are presented and compared. The first method is based on random generation of potential centers for the pebbles, followed by rejection of points that are not compatible with the geometric constraint of no (or limited) pebbles overlap. The second method models the actual physical packing process, accounting for the dynamic of pebbles as they are dropped onto the pebble bed and as they settle therein. A simplification in the latter model is the assumption of a starting point with very dilute packing followed by settling. The results from the two models are compared and the properties of the second model and the dependence of its results on many of the modeling parameters are presented.

KEYWORDS: Pebble-bed reactor, packing, DEM, Molecular Dynamics (MD)

1. INTRODUCTION

The gas-cooled graphite-moderated pebble bed reactor (PBR) concept is a leading candidate for the Next Generation Nuclear Plant (NGNP), a Very High Temperature Reactor (VHTR), under consideration in the US at the Idaho National Laboratory. Similar reactors are actively being designed and planned for construction in the Republic of South Africa and in China. The latter two efforts aim at extensive deployment of these reactors. The efficient and safe operation of these reactors requires the availability of high fidelity, yet computationally efficient, modeling tools. One area of particular importance in the modeling of these reactors is the necessity to properly account for the double heterogeneity of the fuel design and its loading in the reactor. This paper addresses the modeling of the fuel packing within the reactor core.

In the pebble bed reactor, the fuel elements, shaped as spheres, are randomly packed within a cylindrical vat or within an annular zone between graphite reflectors in a cylindrical vat. The assessment of the neutronic behavior, and consequently of the safety and of the fuel economy performance, of the reactor depends on the level of fidelity of the modeling of the packing of the pebbles within the core. For example, the accurate computation of Dancoff factors (needed in the generation of diffusion theory parameters) requires the knowledge of the spatial distribution

of pebbles within the core as well as the accurate determination of their proximity to reflectors or fueled region boundaries. The study of depletion and fuel loading patterns requires the knowledge of the pebbles initial packing distribution and subsequent flow paths and flow speeds. Methods for the modeling of packing as well as for the modeling of pebble flow are under development at the INL and Delft University of Technology. In this paper, the methods developed for use in the determination of the packing pattern of pebbles in a PBR are presented. The first method presented here has already been used in a new code to compute Dancoff factors [1], and the second will soon be incorporated into the same code. The second method is expected to be useful in determining the initial pebble packing distribution and then the subsequent flow of pebbles in dynamic situations such as pebble loading and unloading or during shaking events such as earthquakes.

2. BRIEF SURVEY OF PREVIOUS METHODS

The problem of determining the packing fraction of identical spheres in a vat is an old one. The maximum packing fraction of 74.05% was first given by Kepler in his famous conjecture and shown to be correct only recently [2]. This high packing density is similar to a face-centered cubic lattice. Random packing, naturally, would result in lower densities than this maximum. However the definition of random packing is not well established, as discussed by Torquato et al. [3]. In this latter reference a survey of the history of the problem and one of previous modeling efforts are also given. For applications of interest to the pebble reactor the principal methods of interest are discussed below.

A variety of methods have been used to model the packing of spheres. These range from attempts to accurately model the relevant physics with varying degrees of fidelity, to approximations designed for computational speed, but that do not necessarily reflect the physical situation accurately. Which method is used depends on what information is needed from the model, and the degree of fidelity to be used is naturally commensurate with the requirements of the application.. If the modeling of the dynamic behavior, or movement, of the spheres is required, then accurate physical models are necessary. In contrast, for the computation of Dancoff factors, the path history of the pebbles is not relevant, whereas their final resting positions are. Therefore, a method that accurately models the positions of pebbles in a pebble bed, i.e., pebbles spatial distribution, should be sufficient. In contrast, if fuel depletion is the goal, then actual pebble flow paths are needed, and a method capable of keeping track of pebble position history is necessary.

The low fidelity methods have been discussed in a variety of papers. Two of these methods are the rain model and the stable point model. Besides these, one of the methods presented here, which we term the removal or rejection method, is also a low fidelity method. The former two methods are discussed briefly in this section, whereas the latter is presented in the body of the paper. The rain model randomly drops spheres until they hit a sphere on the bottom. This generates a low packing density so, next, the spheres are randomly perturbed with a downward bias. If the new location of a given sphere is not inside any other sphere(s), then it is retained, otherwise, the perturbation is rejected and the process repeated [4]. The stable point model starts with a random distribution on the bottom layer. Then, stable points (where there are at least three different spheres in contact on the bottom of a new sphere) are found and one is chosen (either randomly, or the lowest) at which a sphere is assumed located. The process is then repeated until the bed is filled to the desired height [5].

Physical, higher-fidelity, methods have also been previously developed. Two of these are the compressible spheres and the hard spheres methods. For the compressible spheres method, if two spheres are in contact, the force between them is dependent on the depth by which the spheres overlap. Other forces that are modeled include static and kinetic friction. These forces are then used to calculate the torques and accelerations on each of the spheres. These forces then cause rotation and linear motion that are in turn used to compute the spheres' positions at the next time step [6, 7, 8]. One of the methods developed in this paper falls within this general category.

Another physical, higher-fidelity, method is one that models collisions as discrete events. In this model, N(N-1)/2 pairs of spheres are considered at each time step. The model determines whether a collision will take place and finds the time at which the event occurs. After determining the consequences (i.e. motion alteration, outgoing velocities) of this first pair collision, the algorithm identifies the next pair that will collide and repeats the process [9]. This method allows hard spheres, but as the average distance between spheres decreases, the number of collisions that need to be calculated increases rapidly, becoming computationally impractical long before stable points are reached in an application of the order of magnitude that of the pebble bed reactor.

3. THE REMOVAL AND THE DYNAMIC METHODS

The methods implemented in this work and compared in this paper include a low fidelity removal method and a high fidelity physical method. The latter is slightly simplified to ignore some dynamic features that are not necessary to modeling the packing in the pebble bed reactor. These features are restored in a more complete third model that we use to describe the flow of pebbles. The former two methods are described in turn in this section.

3.1. The Pebble Removal Incremental Method

The Pebble Removal Incremental Method (PRIMe) works by starting with a large collection of random points, and selects a subset of the points that are non-overlapping pebble positions. Figure 1 shows an illustration of this method. The solid circles are the determined positions, and the outlined circles are potential positions that have not yet been checked. The greater the number of initial random points, the tighter the resulting packing will be. For PRIMe, the number of points generated is approximately 100,000 times the number of pebbles that will fit within the vessel. Then, starting from the bottom, one pebble (i.e., one point) is chosen either arbitrarily or based on criteria chosen by the analyst. All points that would lie within the space occupied by that pebble is removed from the collection. Next, a point is chosen immediately outside the zone that has been cleared of points that would result in overlap had they been taken as pebble centers. Then the clearing process is repeated. The removal/choice process is continued until incrementally the entire pebble bed vat is filled with non-overlapping pebbles, and all initial points have either been removed or determined to be acceptable as the center of a pebble. This process has been coded into the subroutine "RandomPack" of the PEBDAN [1] code. To run this algorithm practically, the points generation and the identification of the acceptable pebbles (those retained) are conducted layer by layer. First, the bottom layer is fully treated. Then, points for the next layer are produced, and sorted from lowest to highest, and then they are sequentially checked from lowest to highest to eliminate the points that would result in

overlapping pebbles if they were chosen as pebble centers. This method improves the speed and memory usage. Since the algorithm only needs to search for overlap in only some of the layers (current layer and immediately adjacent lower layer), the speed is improved. Since only one layer worth of the full number of points to be tried needs to be stored in memory, the memory use is greatly decreased compared to the requirement from modeling the entire 100,000 times the number of final pebbles. This method could also be extended on the horizontal direction, but that was not done in the current code.

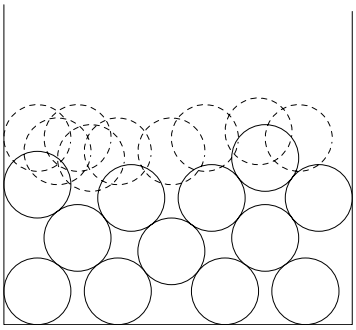

Figure 1. Diagram illustrating the workings of PRIMe

3.2. The Dynamic Pebble Packing Model

The high fidelity physical model method uses a compressible spheres approach. The simulation is initialized with a low-density arrangement where no pebble overlaps another. Each pebble is assigned an initial position, velocity and angular velocity. The time derivatives for each of these variables are calculated and then integrated to determine their subsequent values.

The basic time derivatives for each pebble's variables are:

$$\frac{d\mathbf{v}_i}{dt} = \frac{m_i\mathbf{g} + \sum_{i \neq j} \mathbf{F}_{ij} + \mathbf{F}_{ci}}{m_i} \tag{1}$$

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{v}_i \tag{2}$$

$$\frac{d\boldsymbol{\omega}_i}{dt} = \frac{\sum_{i \neq j} \mathbf{F}_{\perp ij} \times r_i \hat{\mathbf{n}}_{ij}}{I_i} \tag{3}$$

where $\mathbf{v}_i$ is the velocity of pebble i, $\mathbf{p}_i$ is the position of pebble i, and $\boldsymbol{\omega}_i$ its angular velocity. $\mathbf{F}_{ij}$ is the total force on pebble i from pebble j, $\mathbf{F}_{\perp ij}$ is the tangential force on pebble i exerted by pebble j and $\mathbf{F}_{ci}$ is the force of the container on pebble i. The remaining variables are the mass of pebble i, m_i, the radius of pebble i, r_i, the moment of inertia for pebble i, I_i, the normalized vector pointing from pebble i's position to pebble j, $\hat{\mathbf{n}}_{ij}$, and the gravitational acceleration, $\mathbf{g}$. The principal vectors for two interacting pebbles are illustrated in Figure 2.

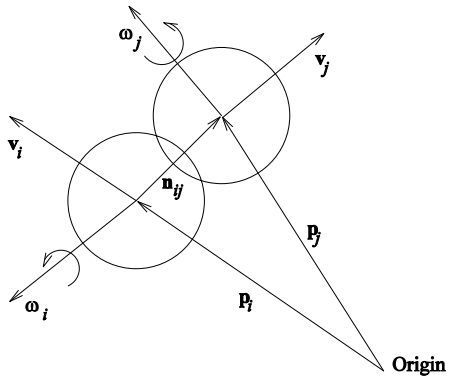

Figure 2. Principal Vectors in the Interaction of Two Pebbles

The contact forces $\mathbf{F}_{ij}$ and $\mathbf{F}_{\perp ij}$ are calculated using Hooke's law, assuming a force linearly proportional to the depth of overlap, and the kinetic friction calculated using a dashpot model following Wait [8]. Therefore, the dynamic forces are given by

$$F_n = hl - Cv_n \tag{4}$$

and

$$F_t = \min(F_n \mu, Cv_t), \tag{5}$$

where F_n is the normal force between pebbles and F_t is the tangential force between them. In the first equation, h is Hooke's law constant, l is the overlap depth of the two pebbles, and v_n is the component of the relative velocity of the pebbles along the line joining their centers. In the second equation, μ is the kinetic friction constant, and C is the dashpot constant, and v_t is the component of their relative velocity normal to the line joining their centers. The combined components of this force are used for calculating the acceleration, and the tangential force is used for calculating the torque.

The relative velocity is calculated as the difference between the surface velocities at the center of the region of contact. The surface velocity combines the translation velocity of the pebble, and the speed at which it is rotating. The formula for calculating relative velocity is:

$$\mathbf{v}_{ij} = (\mathbf{v}_i + \boldsymbol{\omega}_i \times r_i \hat{\mathbf{n}}_{ij}) - (\mathbf{v}_j + \boldsymbol{\omega}_j \times r_j \hat{\mathbf{n}}_{ji}) \quad . \tag{6}$$

The container forces are calculated as if the surface was a pebble with zero velocity and angular velocity with the normal direction between the two taken as perpendicular to the surface of the container.

The weight of each pebble is taken into account in the determination of the balance of forces that act on it. The effect of the weight is to drive the pebbles downward and therefore to increase the packing density or equivalently to decrease the amount of void within the pebble bed. The dashpot friction forces are used to dissipate the initial gravitational potential energy, as the pebbles are allowed to settle in the model. Static friction is treated approximately in the case of

pebbles moving together while remaining in contact. Another approximation relates to the kinetic friction for pebbles in contact with the wall or physical boundary of the pebble bed. For these pebbles, static friction is assumed present between them and the wall if their velocity relative to the wall is below a pre-set model threshold (that can be adjusted as desired). Similarly, if two pebbles are in contact (i.e., the distance of their centers is less than two pebble radii), and if their relative velocity is below the threshold, then static friction is assumed present between them. However, static friction in this latter case is ignored for pebble pairs with large velocity with respect to the wall, as their next collisions will be overwhelmingly governed by other dynamic artifacts. The effects of modeling or ignoring the static friction for these cases are shown in Table I.

Table I. Effect of Static Friction Approximation for Moving Pebbles

	Packing Fraction		
	Without Static Friction	Including Static Friction Approx.	Relative Difference (%)
Including Torque	0.6224	0.6213	0.19%
Without Torque	0.6153	0.6093	0.99%
Relative Difference (%)	1.14%	1.93%	

As the table demonstrates, the effect of static friction on the packing fraction is low, since the inclusion of the static friction approximation results in a mere 0.19% decrease in the packing fraction. With the exception of the results in this table, the dynamic simulation data presented in this paper are for cases with the static friction approximation disabled. Although this not fully rigorous for dynamic calculations, this omission is of little or no consequence in determining final stable locations. This is because the existence of such positions is made possible and is determined by the presence of the static friction, which is modeled for slow moving pebbles as they are settling down. As the comparative packing fractions table demonstrates, the addition of torque increases the packing fraction by 1 to 2%. If speed of simulation is more important than accuracy of fidelity, the torque can be turned off, since it has a low effect on the outcome.

A naïve method of finding pebbles that are in contact would be to search through all the pebbles for pairs within two radii of each other. With such a method, however, the amount of time spent on processing increases as the square of the number of pebbles. The approach implemented in this work (illustrated in Figure 3) avoids this extensive search by partitioning the domain into cubic zones of sides equal to two radii and searching (at the start of each time step) only within a zone and the ones adjacent to it and repeating for all zones. Thus, instead of checking all other pebbles for interaction with the one under consideration, only the pebbles in the nearby zones are checked. Since there is a bounded number of pebbles in each zone, and there is a bounded number of zones that a given pebble could interact with, the time spent processing each time step increases linearly with the number of pebbles, which greatly speeds up the computation when large numbers of pebbles are being processed. The overall computation time is slightly higher

than linear since an increase of the number of pebbles in the model results in a lower fraction of the computations being effectively treated within the cached portions of memory. In addition, an increase in the size of the problem results in fewer boundary zones being part of the computational model and therefore higher overall computational times (boundary zones involve fewer interactions as there are no pebbles on one of their sides).

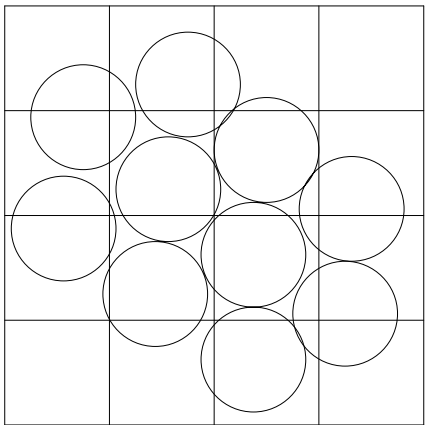

Figure 3. Example of Interaction Zones

4. RESULTS

The results for the two modeling approaches presented in this paper compared to the experimental results of Benenati and Brosilow [10]) are shown in Figures 4 and 5.

Despite its simplicity, the removal method gives remarkably accurate results. As shown in Figure 4, the model yields an average packing fraction of 0.60, which is very close to the experimental packing fraction of 0.61. This method also results in no overlap of the spheres, which is impossible to achieve for compressible sphere methods. However, it is important to bear in mind that in reality, all physical spheres are at least slightly compressible, but realistic compression levels are time-consuming to simulate, so in models that allow compression spheres are made unrealistically soft as discussed by Kohring [6]. The removal method also displays significant similarity to the experimental data with regard to the packing fraction boundary oscillatory behavior, albeit with slightly more rapid dampening of the boundary density fluctuations.

In Figure 5, the dynamic simulation method results are compared to the experimental data. The simulation accurately reproduces the behavior seen in the experimental results. The model packing fraction is 0.61. The boundary density fluctuations dampen out at essentially the same rate as in the experimental data. In contrast to the removal method, the dynamic method allows the spheres to overlap. However, the amount of overlap is relatively small and likely of no consequence on the fidelity of neutronic modeling applications. For example, the maximum overlap for a 27,000-pebble run was less than 2% of a sphere radius, and the average was less than 0.5%. The dynamic method is about an order of magnitude slower than the removal method since it has to repeatedly iterate until the positions are stable.

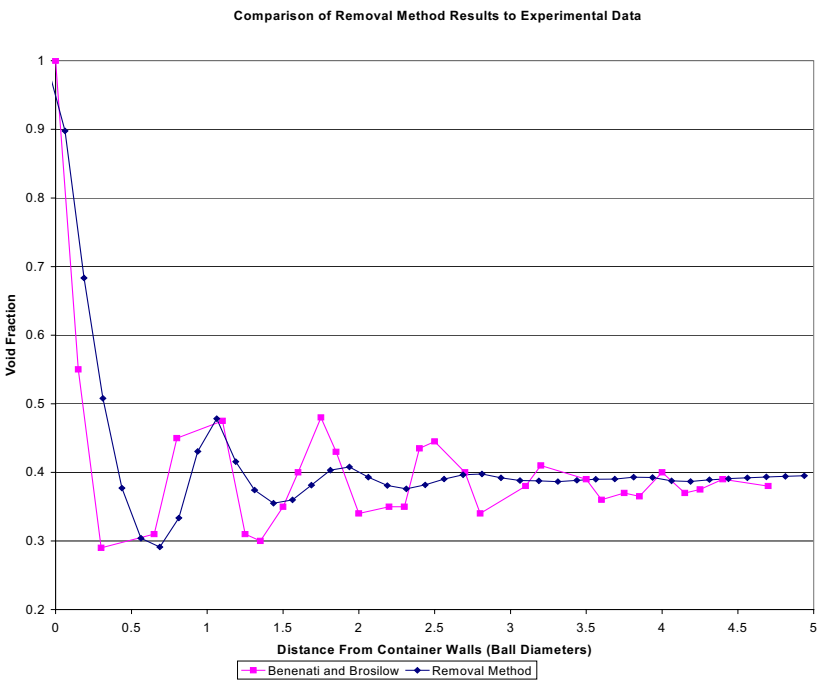

Figure 4. Comparison of Removal Method Results to Experimental Data

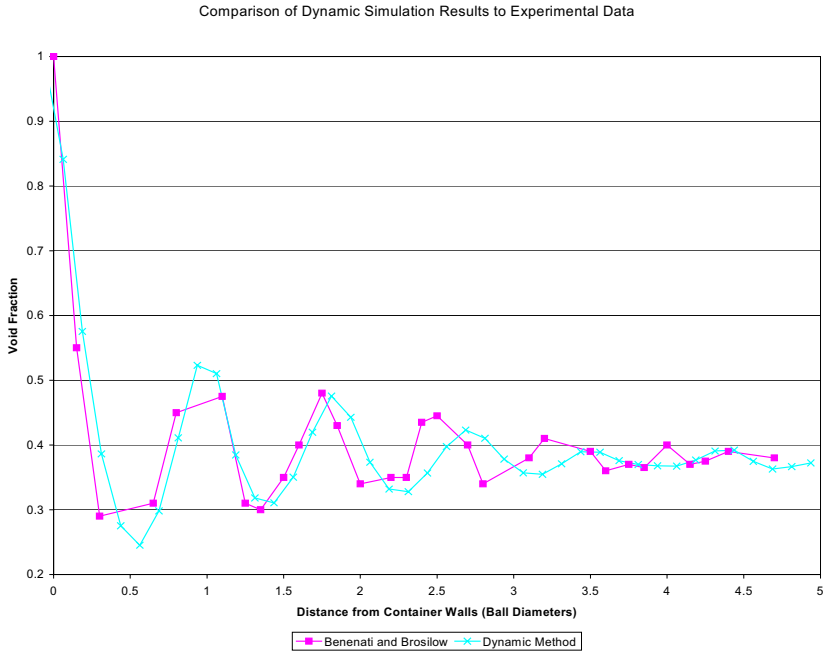

Figure 5. Comparison of Dynamic Pebble Method to Experimental Data

The dynamic model method is more realistic in its representation of the physical behavior of the pebble bed, but the removal method is faster. The codes in which they are embodied may be

combined in order to gain the advantages of both methods. If the removal method is used to generate an initial condition with an extra gap between the spheres, the dynamic method could then be used to model the further compression of the pebble bed to realistic packing fractions.

5. CONCLUSIONS

It is demonstrated in this work that the packing of pebbles in a PBR can be simulated accurately. The level of fidelity in the results depends on the number of features that are simulated. From the results obtained in this work, it is clear that the higher fidelity of the dynamic model results in a more realistic representation of the pebble packing than is achieved with the removal method. In addition, the dynamic model can, and will be, used to model the flow of pebbles subsequent to the initial packing. Both methods could be used in tandem in order to speedup simulations, with one used for providing initial conditions and the other for carrying out the modeling to its conclusion.

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